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Workshop on Science of Wear

September 16-19, 2018 Tsinghua University, Beijing, China

International Workshop on Science of Wear

Program & Abstract

September 16−19, 2018
Tsinghua University
Beijing, China

International Workshop on Science of Wear

September 16−19, 2018

Venue: Lee Shau Kee Science & Technology Building, Tsinghua University, Beijing, China

PROGRAM

September 16, Sunday
14:00—19:00, Registration, Room A505-2
17:00—19:00, Round table discussion, Room A507

September 17, Monday
Room A404

7:30—8:30	On-site registration
8:30—8:40	Opening address Prof. Yonggang Meng, SKLT, Tsinghua Univ., China
8:40—9:20	Rabinowicz criterion for adhesive wear: History and applications Prof. ValentinL. Popov, TU Berlin, Germany
9:20—9:50	Adhesion and deformation in friction transfer and wear Prof. N.Myshkin, MPI, Belarus
9:50—10:20	Toward mechanistic understanding of tribochemical wear Prof. Seong H Kim, Penn. State Univ., USA
10:20—10:40	Coffee break
10:40—11:10	Nanomanufacturing of Si (100) surface at the atomic scale via mechanochemical reactions Prof. Lei Chen, SWJU, China
11:10—11:40	Tribology in hot sheet metal forming Prof. Braham Prakash, Luleå Univ. of Tech., Sweden
11:40—12:10	Computational modeling and experiments of hot metal forming lubrication Prof. Anh Kiet Tieu, Univ. of Wollongong, Australia)
12:10—13:30	**Lunch time**

September 17, Monday
Room A404

13:30—14:00	Numerical methods for the simulation of deformations and stresses in turbine blade fir-tree connections MSc. Justus Benad, TU Berlin, Germany
14:00—14:40	Energy based wear particle prediction with application in automotive tyres Dr. Roman Pohrt, TU Berlin, Germany
14:40—15:10	Surface roughness evolution in atomistic simulations of adhesive wear: from asperity collision to three-body configuration MSc. Enrico Milanese, EPFL, Switzerland
15:10—15:40	Molecular-dynamic study of the influence of size parameter and temperature of the system on adhesive wear mechanisms Prof. Andrey Dmitriev, Russian Academy of Sciences
15:40—16:00	Coffee break
16:00—16:30	Failure mechanisms of graphene for tribological applications (Prof. Qunyang Li, SKLT, Tsinghua Univ., China)
16:30—17:00	Molecular dynamics simulation of atomic-scale wear Prof. Tianbao Ma, SKLT, Tsinghua Univ., China
17:00—17:30	Observation of structural superlubricity in graphite flakes assembled under ambient condition Prof. Ming Ma, SKLT, Tsinghua Univ., China
18:30—20:30	**Workshop banquet**

September 18, Tuesday
Room A404

8:30—9:10	Structure evolution behind the wear behaviors of hydrogenated amorphous carbon films Prof. Junyan Zhang, LICP, CAS, China
9:10—9:40	Modelanalysis of dynamicsliding friction and heat generation on dry inclines Prof. Kazuo Arakawa, Kyushu University, Japan
9:40—10:10	Friction and wear rate of lubricated point contacts during normal running-in processes Prof. Yonggang Meng, SKLT, Tsinghua Univ., China
10:10—10:30	Coffee break
10:30—11:00	The nature of atomic wear Prof. Yunfeng Shi, RPI, USA
11:00—11:30	Wear models for axially symmetric contacts – an overview MSc. Emanuel Willert, TU Berlin, Germany
11:30—12:00	Energy dissipation in contact of functionally graded spherical bodies transmitting tangential forces Dr. Markus Heβ, TU Berlin, Germany
12:00—13:30	Lunch time
13:30—14:00	Sliding friction in junctions of layered materials Prof. Michael Urbakh, Tel Aviv Univ., Israel
14:00—14:30	Wear out failure early-warning of solid lubricating materials by compositing triboluminescent powders Prof. Zhaofeng Wang, LICP, CAS, China
14:30—15:00	Tuning interface nanostructures of polymer-metal rubbing pairs towards ultralow friction and wear Prof. Ga Zhang, LICP, CAS, China
15:00—15:30	Wear and kinetics of friction of heterogeneous composite structures Dr. Qiang Li, TU Berlin, Germany
15:30—15:50	Closing remarks Prof. Valentin L. Popov, TU Berlin, Germany
15:50—16:00	Break
16:00—17:30	**SKLT Lab tour**
18:00—20:00	**Dinner**

September 19, Wednesday
Free discussions/City tour

Notes
1) No registration charge for all presenters and participants;
2) Presenters and participants pay their own travel and accommodation expenses;
3) The host (SKLT) provides meeting room, lunch, coffee break and dinner.

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Venue: Lee Shau Kee Science & Technology Building, Tsinghua University, Beijing, China

ABSTRACTS

Oral presentations

Rabinowicz criterion for adhesive wear: History and applications

Valentin L. Popov

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Abstract: 60 years ago, in 1958, Ernest Rabinowicz published a 5 page paper titled "The effect of size on the looseness of wear fragments" where he suggested a criterion determining the minimum size of wear particles. The criterion of Rabinowicz is based on the consideration of the interplay of elastic energy stored in "asperities" and the work of separation needed for detaching a wear particle. He was probably the first researcher who explicitly emphasized the role of adhesion in friction and wear. In a recent paper in Nature Communications, Aghababaei, Warner and Molinari confirmed the criterion of Rabinowicz by means of quasi-molecular dynamics and illustrated the exact mechanism of the transition from plastic smoothing to formation of wear debris. This latter paper promoted the criterion of Rabinowicz to a new paradigm for current studies of adhesive wear. The size arguments of Rabinowicz can be applied in the same form also to many other problems, such as brittle-ductile transition during indentation, cutting of materials or ultimate strength of nano-composites.

The new understanding of the old Rabinowicz' criterion for adhesive wear opens new possibilities for understanding and numerical simulation of both the coefficient of adhesive wear and the size distribution of wear particles. In the present talk, further generalizations of the Rabinowicz idea are discussed, in particular in application to contacts of complex configuration and to the problem of determining the size distribution of wear particles. On the other hand, we discuss the implications of the Rabinowicz logic for heterogeneous media (coated or having surface layers due to mechanochemical reactions).

Keywords: adhesion; plasticity; wear; Archard's law of wear; Rabinowicz criterion; surface topography; history of tribology

Adhesion and deformation in friction transfer and wear

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Abstract: Theory of friction was developed in two aspects: mechanical (deformation) and molecular one (adhesion). Its history was developed since Archimedes and Leonardo. Still the general theory is not completed even the great mechanicals and physicists have tried. The reason is the complexity of friction phenomena and its multi-scale nature. We are always balancing at the border of continuum mechanics at macroscopic scale with surface physics at atomic-molecular scale.

Surface geometry and nominal normal load are considered as the key factors determining the contact mechanics and deformation in a tribosystem, but contact area and pressure definitions are scale-dependent. Adhesion (surface forces) is another key scale-dependent factor and it strongly affects friction and wear. Origin of surface forces is a combination of phenomena acting at various scales and being of different physical nature.

Mass transfer and wear are related to dominant factors in friction. Commonly fatigue wear is considered to be most affected by concentrated cyclic deformation in the surface layers of material in friction, crack propagation, and wear debris formation. Adhesive wear is controlled by both plastic deformation and surface forces affecting mass transfer in friction and formation of intermediate layer (third body) in the contact. Erosion and abrasive wear are attributed to micro-cutting affected by shear strength of material, geometry of abrasive and normal load.

Theoretical analysis of wear and calculation of wear intensity is a difficult problem and it is solved only in particular cases, e.g. in case of cyclic fatigue wear in rolling bearings where the long-life of the components can be predicted with high accuracy basing on the number of loading cycles, contact pressure and strength of materials in contact. In most practical cases the engineers should relay on the friction and wear tests of different scale – from laboratory to bench testing and further to accelerated full-scale tests under severe operating conditions. The engineering experience has shown that successful wear tests can provide visible practical effect in tribology achieved in recent years with the billions of dollars in GNP savings for industrial economies.

At the current stage it is reasonable to consider the practical engineering problems in tribology with taking account the scale of the problem and previous experience in design of the similar systems fixed in the handbooks and data bases. The common sense and the ancient "Okham's razor": *"Entities must not be multiplied beyond necessity"* -- can be very useful.

Toward mechanistic understanding of tribochemical wear

Seong H. Kim[1,2]

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Abstract: Mechanochemisty is the subject studying chemical reactions initiated or facilitated by mechanical stresses. Chemical reactions occurring at shearing interfaces are specifically called tribochemistry. Compared to thermal, photochemical, and electrochemical reactions where the initial activation of reactant molecules over the energy barrier or transition state is relatively well understood, mechanistic understanding of tribochemical reactions is not well established. One of the significant questions in tribochemical mechanisms would be how mechanical energy is channeled into chemical reaction coordinates. This question is related to the magnitude of the "critical activation volume" which can be obtained from Arrhenius-type analysis of the load or shear stress dependence of reaction yields or rates. This talk will focus on the effects of chemical structures of the adsorbed molecules as well as surface chemistry of shearing interfaces on critical activation volume, which could provide further insights into the physical nature of the critical activation volume.

Nanomanufacturing of Si (100) surface at the atomic scale via mechanochemical reactions

Lei Chen[1], Jialin Wen[2], Tianbao Ma[2], Xinchun Lu[2], Seong H. Kim[1], Linmao Qian[1]

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Abstract: Ultra-precision of nanomanufacturing process down to the atomic level is of paramount importance for new development of nanoelectronics with unique functionalities. The ultimate precision that can be achieved on the crystalline lattice would be the topographic control down to a single atomic layer. Achieving such an ultimate precision requires physical means or processes to reliably and reproducibly remove atomic layers at a specific location with an arbitrary shape without causing subsurface damages or disorders. Here, we demonstrate a SPM tip-based, mask-free and chemical-freelithographic process producing topographic features into the Si (100) surface. This process is based on mechanochemical reactions involving silicon atoms at the topmost surface of the substrate, water molecules adsorbed from the ambient air, and hydroxyl groups at the counter-surface. By controlling the contact scan condition, it is possible to attain the precision down to removal of single atomic layer of silicon which would be the ultimate resolution in the depth direction in topographic patterning on the Si (100) surface. Since the chemical reactions involve only the topmost atomic layer exposed at the interface, removal of the single atomic layer is possible and the crystalline lattice beneath the processed area remains intact, keeping perfect crystalline order without subsurface structural damage. Molecular dynamics simulations were used to explain the atom-by-atom removal process, where the first atomic layer is removed preferentially through the formation and dissociation of interfacial bridge bonds. This mechanochemistry associated manufacturing approach might be applicable to other substrates, such as, GaAs for fabrication of the site-controlled nanopatterning and 2D materials for layered removal. This study opens up a new opportunity for achieving the ultimate precision nanofabrication and reveals the potential for combining the mechanochemistry and SPM scanning to advance the ultra precision nanomanufacturing processes.

Tribology in hot sheet metal forming

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Abstract: The increasing demand for light-weight components, especially in the automotive and transportation sector, is the driving force for the rapid expansion of hot sheet metal forming technologies. In automotive industry, a large number of safety and structural components for the body-in-white are formed using press hardening. This process allows forming of complex shapedcomponents while controlling their microstructure and mechanical properties. Tribology plays an important role in this process as it affects thedurability of forming dies and tools, quality of the produced parts and the overall productivity. The tribological challenges include: friction control, enhancement of the durability of forming tools; minimization/alleviation ofgalling of tools andsurface damage on the produced parts.

This talk focuses on recent tribological studies pertaining to press hardening undertaken by the group at Luleå University of Technology in recent years. The objectives of these studies have been to investigate the effect of tool surface roughness and surface engineering on the friction and wear response. Further, the influence of tool steel composition and tool temperature has also been investigated.The experimental work was carried out using a hot strip tribometer capable of simulating the tribological contact conditions in the press hardening process.

The results have shown that the frictional stability is contact pressure dependent in case of uncoated tool steel and uncoated ultra-high strength boron steel (UHSS). A high contact pressure resulted in more stable friction behaviour. In case of Al-Si coated UHSS, the tool steel surface roughness was found to directly affect the material transfer. A rough surface resulted in increased galling. Hard PVD coatings (AlCrN) were prone to severe adhesive wear and unstable friction whereas post-oxidised plasma nitrided tool steel resulted in minimal galling and stable friction. The chemical composition of uncoated tool steels was also found to have an effect on friction and material. Oxidation of the tool steel during heating resulted in stable friction behaviour due to formation of transfer layers consisting of oxidised debris and Al-Si fragments. This effect was more pronounced for some tool steels. The temperature of the work-piece material was also found to influence the frictional stability and the wear mechanisms in case of tool steel - Al-Si coated UHSS. In general, severe material transfer and high friction was observed at the highest temperature of the work-piece material (~900 ˚C) due to surface melting of the Al-Si coating and degradation of mechanical properties.

Keywords: press hardening; friction; wear; material transfer; hot strip tribometer

Computational modelling and experiments of hot metal forming lubrication

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Abstract: Metal rolling processes are characterised by a combination of large plastic deformation, significant tribological factors and complex loading modes. In the particular case of hot rolling process, the surface of work roll is initially heated up to 650 ^{o}C while in contact with hot steel strips for 10^{-2} -10^{-3} s, and subsequently cooled by water to around 50 ^{o}C during the same cycle. The work-roll surface are subjected to high loading (10 m/s), the work-roll surface inevitably degrades (e.g. oxidation, wear, abrasion, fatigue, etc.). The metal deformation is closely related to the friction and lubrication conditions between the roll and the material surfaces.

The lubricant composition can affect the friction and dynamics of the rolling process. At the strip-lubricant/roll interface, tribology has a significant influence on the roll wear, the dimensional accuracy and the surface quality of strip in terms of the mechanical and metallurgical properties. The presentation will cover the tribological evaluation of inorganic polymeric compounds build a hierarchical boundary film during hot rolling of steel against wear and friction by using multi-scale advanced characterization techniques, and the tribochemical interaction of an inorganic glass lubricant (phosphate, borate and silicate) and metal/oxide surfaces are performed on the basis of the density functional theory (DFT) and first principles molecular dynamics (FPMD) studies to obtain the tribological dynamics and mechanics of high temperature lubricants.

Numerical methods for the simulation of deformations and stresses in turbine blade fir-tree connections

Justus Benad
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Abstract: The rotating components in a gas turbine are a challenge for both design and manufacturing. Especially turbine blades lead the way in terms of future technology. Improvements of these components may result in a lower weight, an increased turbine performance, a longer life, and lower operating costs. For aero engines, such improvements have a positive impact on the entire aircraft. Among the most critical parts of the turbine are the fir-tree connections of turbine blade and turbine disk. The loads in these connections strongly influence the living of blade and disk. In this work, different numerical methods for the simulation of deformations and stresses in turbine blade fir-tree connections are examined. The main focus is on the Method of Dimensionality Reduction (MDR), the Boundary Element Method (BEM) and the Finite Element Method (FEM). Generally, fir-tree connections require a computationally expensive finite element setup. Their complex geometry exceeds the limitations of the faster numerical techniques which are used with great success within the framework of the half-space approximation. Ways to extend the range of application of the MDR and the BEM to the particular problem of the highly undulating surfaces of the fir-tree connection will be shown and discussed.

Energy based wear particle prediction with application in automotive tyres

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Abstract: Wear particles in engineering system are generated in different sizes, depending on the tribological contact in general, on the contacting surface topographies and on material properties of the worn partner. The size distribution of particles is of great importance for the relevance of the particles after they are emitted from the contact. It determines their toxicity, how and where they are transported and how well they can be degraded biologically.

With a special emphasis on the particles found in road dust, we discuss recent advances in predicting the sizes of wear particles in a given tribological system.

Using Boundary Elements Simulation, we demonstrate how the availability of stored elastic energy can be checked such that deterministic particle locations and sizes are identified.

The theoretical foundation is the idea of Rabinowicz [1], recently reinterpreted be Aghababaei et al. [2] and generalized to general contact zones by Popov [3].

We show that the type of surface interaction (adhesive, fry friction, etc…) strongly influences the feasibility of particles to emerge.

With an energy based approach likes ours, the “large particle paradox” arises: Why do we not see very large wear particles in nature? Last we discuss how to deal with this problem.

References

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Surface roughness evolution in atomistic simulations of adhesive wear: From asperity collision to three-body configuration

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Abstract: Surface roughness is relevant to all the phenomena and processes that take place at the interface between two bodies, like adhesion, contact, friction, and wear. Understanding the relation between surface roughness evolution and wear is therefore key in several fields: from the optimization of the design of manufactured objects to the understanding of fault slip during earthquakes. Experimental evidence and field observation show that worn surfaces are self-affine[1,2]. The complexity of the wear phenomenon makes the understanding of the underlying physics a challenge though, and complicates the quest for simplified, yet sufficiently accurate models capable of describing the wear process. The same reason does not make numerical modeling simple either, as continuum approaches cannot capture the aforementioned complexity, while discrete approaches are limited by the computational cost necessary to investigate length and time scales relevant to engineering applications.

A recently developed atomistic simulations approach[3] permitted us to overcome the length-scale limitation. This allowed us to gain significant insights on the physics of surface roughness evolution during adhesive wear processes. Our results show that the evolution of the surface morphology can be split in two different phases: running-in and long-term sliding. In the first phase, two surfaces come into contact at the asperity level. We find[3] that a material-dependent critical length scale governs the ductile-to-brittle transition: if the junction formed by the two colliding asperities is smaller than this critical length, the asperities deform plastically, otherwise they break. This is a fundamental turning point for the surface roughness evolution: if no junction is large enough, the surfaces will smooth continuously until they weld together. On the contrary, when the junction size is sufficiently large, a debris particle is formed by fracture, thus creating roughness.

The evolution of the surface roughness after running-in is characterized by a different configuration. In our simulations, the debris particle formed upon the initial contact is constrained to roll between the two surfaces and the system transitions to a three-body configuration. The changes in the morphology are then governed by the contact between the debris particle and the surface. Over long time-scales, this leads the worn surfaces to exhibit a self-affine morphology.

In this presentation we will also address the relation between tangential work and wear volume[4] and the interaction between multiple asperities at the onset of wear[5].

Keywords: surface roughness; adhesive wear; atomistic simulations; third body

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scale of micro-fractures to the scale of continents. Geophys. Res. Lett. 40, 83-87 (2013).
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Molecular dynamics study of plastic ploughing of nano-sized polycrystalline titaniumunder scratch testing

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Abstract: The processes of nucleation and development of plastic deformation in a nano-sized titanium polycrystal subjected to scratching are in the focus of this paper. For this aim the molecular dynamics method is used. It is established that the development of plastic deformation as well as the mechanical properties and the residual depth of scratch grooves of individual grains are determined by the difference in their crystallographic orientations. The mechanisms of plastic ploughing of the material during the passage of the indenter through grain boundaries and twin boundaries are also analyzed. It is shown that the internal borders play an important role not only as a barrier to dislocation movement, but also contribute to the manifestation of rotational deformation modes. The simulation results show a good qualitative and, in some cases, a quantitative agreement with the available experimental data.

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Failure mechanisms of graphene for tribological applications

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Abstract: Recent experiments have shown that graphene preserves a superior lubrication property at the nanoscale even with its thickness down to a few atomic layers. Despite the nearly "perfect" properties exhibited at the nanoscale, the tribological performance of graphene at the macroscale is often less satisfactory or even disappointing. To better understand the mechanical properties of graphene and reveal the mechanisms that dictate this scale dependent tribological behavior, we performed a series of atomic force microscopy (AFM) scratch tests to characterize the wear resistance of graphene and we used molecular dynamics (MD) and finite element (FE) simulations to reveal the wear mechanisms.

Molecular dynamics simulation of atomic-scale wear

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Abstract: It has long been a challenge to capture the wear behaviors at the buried sliding interface, especially with atomic resolution, where molecular dynamics simulation provides a promising solution. Here, I will introduce our recently work about molecular dynamics simulation of atomic-scale wear.

Firstly, the wear mechanism of graphene has been investigated by using a modified REBO potential proposed by Pastewka and Moseler et al. The graphene coating on both of the sliding surfaces can greatly increases the critical normal load for wear of graphene. The suppression of nanoscale wear is attributed to the weakening of the atomic interlocking with atomically smooth graphene/graphene sliding interface. Also the effects of the number of graphene layers and the defects on atomic scale wear have been elucidated.

Secondly, the tribochemical wear of silicon, reflecting the materials removal mechanism during the chemical mechanical polishing process has been studied by using the reactive molecular dynamics simulation with the forcefield fitted by DFT calculations. We show that the tribochemical wear can be described by interfacial Si-O-Si bond forming and breaking, where the materials removal rate increases with the normal pressure due to the increase in the number of interfacial bridge bonds. Furthermore, the atom-by-atom removal process has been simulated, where the first atomic layer of Si (100) surface is removed preferentially.

Observation of structural superlubricity in graphite flakes assembled under ambient condition

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Abstract: To date structural superlubricity in microscale contacts are mostly observed in intrinsic graphite flakes that are cleaved by shearing from HOPG mesas in situ or friction pairs assembled in vacuum due to the high requirement of ultra clean interface for superlubricity, which severely limits its practical application. Here we report observation of microscale structural superlubricity in graphite flake pairs assembled under ambient condition where contaminants are inevitable present at the interfaces. For such friction pairs, we find a novel running-in phenomenon, where the friction decreases with reciprocating motions but no morphological or chemical changes can be observed. The underlying mechanism for the new running-in process is revealed to be the removal of third bodies confined between the surfaces. Our results expand the understandings of microscale superlubricity and may help to extend the application of superlubricity in practice.

Structure evolution behind the wear behaviors of hydrogenated amorphous carbon films

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Abstract: Carbon has several allotropic forms capable of creating a variety of nanocarbons with nanoscale size shapes, such as graphene, nanodiamonds, fullerenes etc. When these nanocarbons are introduced in the a-C:H films, the formed short- or medium-range ordered structures can lead to many extraordinary properties. However, the nanostructure films are studied separately and their structure effects on sliding-induced interface changes and surface wear has never enjoyed elaboration. Here, the wear behaviors at the macroscale, and the nanostructure evolutions behind them for carbon films (such as fullerene-like and graphite-like carbon (sp^2-rich), and nanodiamond (sp^3-rich) are reviewed and discussed with the choice of counterface materials and environments, in order to promote the development and application of the films and give helpful guidance for future research, for example, in terms of microstructure design and performance manipulation for the films.

Keywords: wear; friction; a-C:H; fullerene-like; graphite-like; nanodiamond

Model analysis of dynamic sliding friction and heat generation on dry inclines

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Abstract: An analytical model is proposed for dynamic sliding friction and heat generation at the interface between steel pin samples and thermal paper inclines. The dynamic friction was described as $F_d = Av$, where is a parameter related to the surface conditions, A is the contact area and v is the sliding velocity. Analytical expressions are derived for the sliding velocity and frictional shear stress at the interface. The applicability of the model is examined by comparing the experimental velocities and temperature change determined for the samples on the paper surfaces. The model predicted all of the important qualitative features of the velocity and temperature change during the sliding process.

Keywords: Analytical model; dynamic sliding friction; sliding velocity; heat geration; compression and shear stress; steel pin and thermal paper

Friction and wear rate of lubricated point contacts during normal running-in processes

Yazhao Zhang, Alexander Kovalev, Yonggang Meng
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Abstract: The combined effect of boundary layer formation and surface smoothing on friction and wear rate of metallic surfaces under lubricated point contact condition was investigated. The double trend of friction coefficient variations was revealed during running-in and sub-running-in processes. The evolution of surface topography was measured on-site using white-light interference profilometer and analyzed using bearing area curves. Comprehensive theoretical equations that explicitly express the contributions of boundary friction, adhesive friction and wear have been derived, and results obtained by these equations were compared with experimental observations. It is concluded that the theoretical models are quantitatively adequate to describe the combined effect of surface smoothing due to mechanical wear and formation of boundary films on the changes in friction and wear rate during normal running-in processes.

The nature of atomic wear

Yunfeng Shi

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Abstract: We present a systematic study of single-asperity tip wear on flat substrate using molecular dynamics simulations. There are two dominate wear modes observed: the linear plastic wear regime (high stress, high adhesion and no/low lubrication), and the highly non-linear atomic wear regime (low stress, low adhesion and lubricated interface). We further illustrate the nature of the atomic wear in terms of stress-dependency, temperature-dependency, sliding-velocity-dependency, as well as apparent size-effect. These results are crucial to understand the nature of the activation mechanism of atomic wear, which must be determined prior to quantitative wear law for the atomic wear regime.

Wear models for axially symmetric contacts – an overview

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Abstract: The incorporation of wear into classical contact mechanics is a longstanding and non-trivial task in technology. Thereby the wear dynamics and the contact problem often cannot be studied separately of each other, but rather form the strongly coupled wear-contact-problem. A very prominent example for this is fretting. The difficulties encountered when dealing with wear-contact-problems are manifold: wear is an extremely complicated multi-physical-chemical process, whose dynamics can hardly be captured in terms of a general, simple, mathematical law, the "pure" (elastic, elastic-plastic, viscoelastic etc.) contact problem itself may be complicated to solve or the time-scales of the contact problem and the wear process may be very different (the list could easily be continued).

The report will be roughly divided into three parts. First an overview will be given about several experimentally and theoretically obtained wear laws under different circumstances. The wear law together with the kinematics and the constitutive contact-mechanical relations between (surface) stresses and displacements form the mathematical framework of the wear-contact problem. Thus, in a second part, the fully transient dynamics of contact wear are demonstrated for some very simple yet technically relevant problems involving an elastic half-space or a thin elastic layer. Nonetheless, in many cases not the complete transient process (whose precise description may be utterly complicated) is of interest, but only a stationary state (whose determination is usually much simpler) eventually reached after the wear process. The third section of the report will therefore deal with some stationary solutions of wear-contact problems, including the limiting profile shape after fretting and others.

Energy dissipation in contact of functionally graded spherical bodies transmitting tangential forces

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Abstract: The use of functionally graded materials (FGM) within modern technological developments has become indispensable. Due to their spatial gradients in composition or structure, FGMs can significantly increase the resistance to contact deformation and damage. It has been demonstrated both experimentally and numerically that a controlled elastic modulus can suppress the formation of cracks during normal indentation and frictional sliding [1]. In order to make qualitative predictions regarding the improvement of contact properties, analytical solutions are extremely important. Unfortunately, they are only possible for a few laws of elastic inhomogeneity. These include power-law graded materials (PLGM), whose elastic modulus changes with depth perpendicular to the half-space surface according to a power-law. However, even for these materials almost only calculations for non-adhesive and adhesive normal contact problems have been made [2],[3]. Heß and Popov [4] only recently developed analytical solutions of tangential contacts between axisymmetric bodies of FGMs. Up until then, merely the plane tangential contact problem between a rigid, infinitely long cylinder and the elastically inhomogeneous half-space was considered completely solved [5].

In this paper, we present select solutions of contact problems between two power-law graded elastic bodies with spherical surfaces transmitting tangential forces. The focus is always on the calculation of energy dissipation and its effects on wear. First, the classical partial slip contact problem of a periodic tangential force at constant normal force is solved. In addition, based on the work of Johnson [6], an extension to the tractive rolling of a power-law graded sphere on a power-law graded half-space will be presented.

Furthermore, the quasi-static response to more general variations in both normal and tangential forces is investigated. In 2015 Popov et al. [7] showed, that even in the case of no slip there is generally some energy loss if the contact passes through a closed cycle of normal and tangential loading. This phenomenon, which can essentially contribute to structural damping, was called ‘relaxation damping’. It provides a good approximation to the energy dissipation in cases that are far from the gross slip limit. Here we analyze the influence of elastic inhomogeneities on relaxation damping.

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Sliding friction in junctions of layered materials

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Abstract: Friction and wear are the two central causes for energy loss and component failure in mechanical systems. Structural superlubricity may provide a viable route to the reduction of friction and wear that relies on the effective cancellation of lateral forces within incommensurate rigid crystalline contacts. In recent years, much attention has been paid to heterogeneous layered materials junctions that may exhibit robust superlubrictity as well as enhanced performance over their homogeneous counterparts.

In this talk I will present results of fully atomistic numerical simulations of static and dynamical properties of graphite/hexagonal boron nitride (*h*-BN) heterojunctions, performed adopting a recently developed inter-layer potential. Our simulations demonstrate that structural superlubricity at interfaces between graphite and *h*-BN persists even for the aligned contacts sustaining external loads. The frictional anisotropy in the heterojunctions is found to be orders of magnitude smaller than that measured for their homogeneous counterparts. The simulations reveal that the underlying frictional mechanisms in the two cases originate from completely different dynamical regimes.

Using atomistic molecular dynamics calculations, we predict a negative friction coefficient in graphite/*h*-BN heterojunctions, where friction is reduced upon increasing normal load. The origin of this counterintuitive behavior lies in the load-induced suppression of the out-of-plane distortions of the moiré superstructure leading to a less dissipative dynamics of the interface.

Further control over the physical properties of 2D layered materials can be gained via tuning the aspect-ratio of nanoribbons. We demonstrate snake-like motion of graphene nanoribbons atop graphene and *h*-BN substrates. The sliding dynamics of the edge-pulled nanoribbons is found to be determined by the interplay between in-plane ribbon elasticity and interfacial lattice mismatch. This results in an unusual dependence of the friction-force on the ribbon's length, exhibiting an initial linear rise that levels-off above a junction dependent threshold value dictated by the pre-slip stress distribution within the slider.

Our results are expected to be of general nature and should be applicable to other van der Waals heterostructures.

Wear out failure early-warning of solid lubricating materials by compositing triboluminescent powders

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Abstract: Lubrication is recognized as the most effective approach to reduce wear, which could enhance the durability of the machine moving parts. As the alternatives of lubricating oils and greases, solid lubricating materials (SLMs) show the advantage of excellent physical and chemical stability, which have been widely applied in engineering. For practical applications, the lifetime of SLMs is crucial adjective, because severe accidents would occur if SLMs are beyond their lifetime (namely wear out failure). In this work, we present an approach to achieve the wear out failure early-warning of SLMs by introducing triboluminescent materials. The typical graphite/epoxy-based SLMs and $SrAl_2O_4$: Eu^{2+}, Dy^{3+} (SAOED) ceramic powders are employed as the lubricant hosts and triboluminescent components, respectively. The tribological results suggest that the introduction of SAOED could not only maintain the friction coefficient and the wear rate of the graphite/epoxy SLMs, but also endow them with intense triboluminescence. Based on these results, a bilayered structure of SAOED/graphite/epoxy self-lubricating bulk material and solid lubricating coating were designed and fabricated, in which intelligent wear out failure early-warning of the SLMs was achieved by monitoring the produced triboluminescence. The developed wear out failure early-warning approach based on TL signals is supposed to be further extended to various SLMs by compositing suitable TL materials.

Keywords: Solid lubricating materials; failure early-warning; triboluminescence

Tuning interface nanostructures of polymer-metal rubbing pairs towards ultralow friction and wear

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Abstract: It has been recognized that tribofilm formation is of great importance for tribological performance of polymer-metal rubbing pairs subjected to dry friction and boundary lubrication conditions. In this work, we characterized comprehensively nanostructures and mechanical properties of tribofilms of several polymer composites rubbed with metallic counterparts. Depending on the molecule structures, polymer chains can break and free radicals generated finally chelate with the metallic counterface, enhancing the adhesion of the tribofilm onto the metal substrate. With respect to the dry sliding of some self-lubrication nanocomposites, the nanofillers released from the bulk composite are tribo-sintered into a compact layer after mixing with remnant polymer debris. Based on the understanding on formation and function mechanisms of high-performance tribofilms, we compounded new species into formulated composites to modify the interface structures. Our work demonstrated that further addition of only low-loading ceramic nanoparticles into a formulated non-asbestos organic brake material directly switched the material's functionality to an extremely wear-resistant self-lubrication material. Comprehensive interface investigations revealed that the dramatic reductions of friction and wear derived from a nanostructured lubricious tribofilm formed in-situ. Tribofilm formation was continuously fed by complex molecular species released from the bulk composites, for which nanoparticles digested within the tribofilm greatly enhanced its robustness.

Wear and kinetics of friction of heterogeneous composite structures

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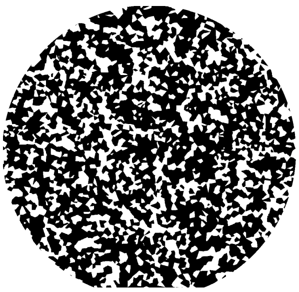
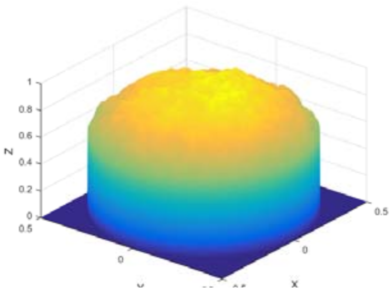
Abstract: The character of roughness and the level of friction in the stationary wear state after long enough "running-in" process are of key importance for numerous applications as e.g. for the friction between tires and road. In the present talk, a method of calculation of surface topography of a multiphasic punch in the stationary worn state is suggested under the assumption of Archard's wear law. The limiting shape is found in the closed integral form andthe obtained solution is applicable to systems with arbitrary number of different phases and arbitrary geometrical in-plane configuration of the phases. A detailed numerical study is carried out for the case of bi-phasic indenters. Figure 1 is an example of biphasic composite.

Using the obtained limiting profiles, the rms slope is determined as a topographic property most directly related to the coefficient of friction. Both simulations and analytical estimations show that the limiting shape does not depend on the "scaling" of the phase structure. The complete set of parameters determining the final state and the limiting rms slope contains: average (apparent) pressure in the contact area, the filling factors (or concentrations) of the phases, and the ratio of the wear coefficients. The obtained result provides a rule for design of composite structures providing the required frictional properties after long running-in.

Experiments on homogeneous and heterogeneous samples are carried out and the results are compared with theoretical predictions. Experimental results show very good qualitative and acceptable quantitative agreement with theoretical predictions.



(a)



(b)

Figure 1: An example of biphasic composite: (a) distribution of two phases with wear coefficient k_2/k_1=10 (white and black); (b) the worn surface topography at the stationary state.

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